

# PLUG

## A PROGRAM FOR THE ANALYSIS OF PLUG-FLOW REACTORS WITH GAS-PHASE AND SURFACE CHEMISTRY

Reaction Design

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*Reaction Design cautions that some of the material in this manual may be out of date. Updates will be available periodically on Reaction Design's web site. In addition, on-line help is available on the program CD. Sample problem files can also be found on the CD and on our web site at [www.ReactionDesign.com](http://www.ReactionDesign.com).*

## PLUG: A PROGRAM FOR THE ANALYSIS OF PLUG-FLOW REACTORS WITH GAS-PHASE AND SURFACE CHEMISTRY

### ABSTRACT

PLUG simulates the behavior of plug-flow chemical reactors. More specifically, the program is designed to model the non-dispersive, one-dimensional flow of a chemically reacting, ideal-gas mixture in a conduit of essentially arbitrary geometry. The program makes use of the CHEMKIN and SURFACE CHEMKIN Utility packages to handle gas-phase and heterogeneous kinetics, as well as species thermodynamic properties. PLUG solves the set of differential/algebraic equations describing the reactor using the implicit numerical software DASSL the set of differential/algebraic equations describing the reactor. These equations are briefly presented here, followed by the procedures for running PLUG. A sample problem includes input and output files for flow in a circular channel, including chemical vapor deposition on the channel walls.



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# 1. INTRODUCTION

Tubular flow reactors have long been used throughout the chemical process industries. The tube flow configuration is a natural choice for processes that are carried out in a continuous fashion. For this reason, such reactors are usually operated at steady state. Traditional applications have included both homogeneous reactions (carried out in an empty tube) and fluid-solid heterogeneous reactions in packed beds. More recently, tubular reactors have been used extensively to deposit thin solid films via chemical vapor deposition (CVD). While this is technically a batch process with regard to the solid deposit, the reactor still operates essentially at steady state for extended periods of time. PLUG is a general model for the steady-state tube flow reactor that can be used for process design, optimization, and control.

Because the general equations for chemically reacting flow involve transport phenomena in addition to kinetics and thermodynamics, rigorous reactor models are by necessity multidimensional. However, there are often practical as well as mathematical reasons for considering idealized models of reduced dimensionality. In the case of tube flow, the accepted ideal is the plug-flow reactor, in which it is assumed that there is no mixing in the axial (flow) direction but perfect mixing in the direction(s) transverse to this. It can be shown<sup>2</sup> that the absence of axial mixing allows the achievable reactant conversion to be maximized. Likewise, the lack of transverse gradients implies that mass-transfer limitations are absent, once again enhancing the reactor performance. Along with these practical advantages, the plug flow reactor is computationally efficient since it is modeled using first-order ordinary differential equations (ODE's), and no transport properties are needed.

The CHEMKIN Application PLUG can be used to analyze plug flow reactors for arbitrary applications involving gases. Like other CHEMKIN Applications, such as SPIN, CRESLAF, and AURORA, it is designed to handle any user-specified gas-phase and surface reaction mechanisms by interfacing with the CHEMKIN and SURFACE CHEMKIN Utility software. PLUG solves the differential/algebraic system of equations using the implicit solver DASSL<sup>3</sup>. Process parameters and solution control options are supplied to the program via Keyword input, and both text and binary solution output files are produced.

In Chapter 2, governing equations for the plug flow reactor are first summarized for reference. Chapter 3 discusses the mechanics of actually running the program and pre-processors and then Chapter 4 discusses the keyword input used in specifying the problem to be solved. Chapter 5 discusses post-processing options. Finally, Chapter 6 gives input files for a sample problem and presents a discussion of the output generated.

## 2. REACTOR EQUATIONS

The equations governing the behavior of the plug flow reactor are simplified versions of the general relations for conservation of mass, energy, and momentum.<sup>4</sup> They can be derived most easily by writing balances over a differential slice in the flow direction  $x$ , with the stipulations that (a) there are no variations in the transverse direction, and (b) axial diffusion of any quantity is negligible relative to the corresponding convective term. In this way the overall mass balance (continuity equation) for the gas is found to be

$$\rho u \frac{dA}{dx} + \rho A \frac{du}{dx} + u A \frac{d\rho}{dx} = a_i \sum_{gas}^{K_g} \dot{g}_k W_k . \quad (1)$$

Here  $\rho$  is the (mass) density and  $u$  the axial velocity of the gas, which consists of  $K_g$  species;  $W_k$  is the molecular weight of species  $k$ , and  $\dot{g}_k$  is the molar production rate of this species by all *surface* reactions. The quantities  $A$  and  $a_i$  are the cross-sectional (flow) area and the internal surface area per unit length, respectively, of the reactor; each can be a function of  $x$ . Equation (1) simply states that the mass flow rate of the gas can change as a result of generation or consumption by surface reactions. A similar equation can be written for each species individually:

$$\rho u A \frac{dY_k}{dx} + Y_k a_i \sum_{gas}^{K_g} \dot{g}_k W_k = W_k (\dot{g}_k a_i + \dot{\omega}_k A) . \quad (2)$$

Here  $Y_k$  is the mass fraction of species  $k$  and  $\dot{\omega}_k$  is its molar rate of production by homogeneous *gas* reactions. Such reactions cannot change the total mass of the gas, but they can alter its composition.

Turning now to the energy equation, one finds

$$\begin{aligned} \rho u A \left( \sum_{gas}^{K_g} h_k \frac{dY_k}{dx} + \bar{C}_p \frac{dT}{dx} + u \frac{du}{dx} \right) + \left( \sum_{gas}^{K_g} h_k Y_k + \frac{1}{2} u^2 \right) a_i \sum_{gas}^{K_g} \dot{g}_k W_k \\ = a_e Q_e - a_i \sum_{bulk}^{K_b} \dot{b}_k W_k h_k \end{aligned} \quad (3)$$

where  $h_k$  is the specific enthalpy of species  $k$ ,  $\bar{C}_p$  is the mean heat capacity per unit mass of the gas,  $T$  is the (absolute) gas temperature, and  $\dot{b}_k$  is the molar production rate of bulk solid species  $k$  by surface reactions. The distinction between bulk and surface species is discussed in the SURFACE CHEMKIN manual. Equation (3) states that the total energy (enthalpy plus kinetic) of the flowing gas changes due to the heat flux  $Q_e$  from the surroundings to the outer tube wall (whose surface area per unit length is  $a_e$ ) and also due to accumulation of enthalpy in the bulk solid. Equivalently, the right-hand side of Eq. (3) can be written as



$$a_i Q_i + a_i \sum_{gas}^{K_g} \dot{g}_k W_k h_k$$

where  $Q_i$  is the heat flux to the gas from the inner tube wall. The methods for handling  $Q_e$  and  $Q_i$  will be discussed below. It is worth noting that Eq. (3) does not involve the enthalpies of the *surface* species.

The momentum equation for the gas expresses the balance between pressure forces, inertia, viscous drag, and momentum added to the flow by surface reactions. Thus

$$A \frac{dP}{dx} + \rho u A \frac{du}{dx} + \frac{dF}{dx} + u a_i \sum_{gas}^{K_g} \dot{g}_k W_k = 0, \quad (4)$$

where  $P$  is the absolute pressure and  $F$  is the drag force exerted on the gas by the tube wall, to be discussed below. The pressure is related to the density via the ideal-gas equation of state:

$$P \bar{W} = \rho R T, \quad (5)$$

where  $R$  is the universal gas constant and  $\bar{W}$  is the mean molecular weight.

Since the heterogeneous production rates  $\dot{g}_k$  and  $\dot{b}_k$  will depend, in general, on the composition of the surface as well as that of the gas, equations determining the site fractions  $Z_k$  of the  $K_s$  surface species are now needed. Assuming that these species are immobile, the steady-state conservation equations are extremely simple:

$$\dot{s}_k = 0. \quad (6)$$

i.e., the net production rate of each surface species by heterogeneous reactions must be zero. There is, however, a complication. In PLUG we assume that the total site density for each surface phase is a constant. As a result, the algebraic equations represented by (6) are not all independent, and for each phase one of the equations must be replaced by the condition

$$\sum_{phase} Z_k = 1. \quad (7)$$

In order to minimize errors, Eq. (7) is used to replace Eq. (6) for the species having the largest site fraction. An analogous relation for the gas phase is not needed, since (2) is a differential (as opposed to algebraic) equation. In fact, by summing Eqs. (2) it can be shown that the  $Y_k$  will automatically add up to unity at each point.

The system of governing equations for the reactor is now mathematically closed. However, because the residence time  $\tau$  of the gas is often a quantity of interest, it is useful to include an equation that computes it automatically. This is simply

$$\frac{d\tau}{dx} = \frac{1}{u}. \quad (8)$$

Equations (1)-(8) provide a total of  $5 + K_g + K_s$  differential/algebraic relations involving the dependent variables  $\rho$ ,  $u$ ,  $T$ ,  $P$ ,  $\tau$ ,  $Y_k$  and  $Z_k$ . The functions  $\bar{W}$ ,  $h_k$ ,  $\bar{C}_p$ ,  $\dot{\omega}_k$ ,  $\dot{g}_k$ ,  $\dot{s}_k$ , and  $\dot{b}_k$  can all be expressed in terms of these and are obtained from calls to CHEMKIN and SURFACE CHEMKIN subroutines. The quantities  $A(x)$ ,  $a_i(x)$ , and  $a_e(x)$  are fixed by the reactor geometry. This then leaves only  $Q_e$ ,  $Q_i$ , and  $F$  to be addressed.

PLUG actually provides five different options for handling the reactor energy balance. First of all, the reactor can be declared to be isothermal, or the (axial) temperature profile can be specified via a subroutine; in either case Eq. (3) is not used. Alternatively, the reactor can be declared to be adiabatic ( $Q_e = 0$ ), or the axial heat flux profile  $Q_e(x)$  can be specified. The final option is to write  $Q_i$  in terms of the ambient temperature  $T_\infty$  and an *overall* heat-transfer coefficient  $U$ :

$$Q_i = U(T_\infty - T). \quad (9)$$

Both  $T_\infty$  and  $U$  must be supplied by the user.

The viscous drag force  $F$  is written in terms of a friction factor  $f$  as follows:

$$\frac{dF}{dx} = a_i \cdot \frac{1}{2} \rho u^2 f. \quad (10)$$

The friction factor can in turn be expressed as a function of the local Reynolds number

$$\text{Re} = \frac{Du\rho}{\mu}, \quad (11)$$

where  $D$  is the tube diameter (or the mean hydraulic diameter for a conduit with a noncircular cross section) and  $\mu$  is the gas viscosity. For laminar flow ( $\text{Re} < 2100$ ) the analytical result for round tubes is

$$f = \frac{16}{\text{Re}}, \quad (12)$$

while for turbulent flow one can use the approximate Blasius formula,<sup>4</sup>

$$f = 0.0791 \text{Re}^{-0.25}. \quad (13)$$

This approach is only approximate, especially for noncircular conduits, but viscous drag is usually of very minor importance in gas-phase reactors. In keeping with this, and in order to avoid having to calculate transport properties, the gas viscosity is computed by scaling the inlet value (supplied by the user) by  $(T/T_{in})^{0.5}$  and ignoring the composition dependence.

It remains to specify the initial (inlet) conditions for the reactor. Clearly, values for  $\rho$ ,  $u$ ,  $T$ ,  $P$ , and  $Y_k$  at  $x = 0$  should be known or easily obtainable from the problem statement, the ideal gas law, and the reactor geometry, and of course  $\tau = 0$  at this point. Since there are no derivatives of the  $Z_k$  in the governing equations, it might appear that no initial conditions are needed for them. However, DASSL requires that all algebraic equations be satisfied at the initial point, so Eqs. (6) and (7) must be solved for the  $Z_k$  using the known values of the other variables. In PLUG this is accomplished in a separate preliminary calculation, in which DASSL is used to integrate the fictitious transient equations

$$\frac{dZ_k}{dt} = \frac{\dot{s}_k \sigma_k}{\Gamma} \quad (14)$$

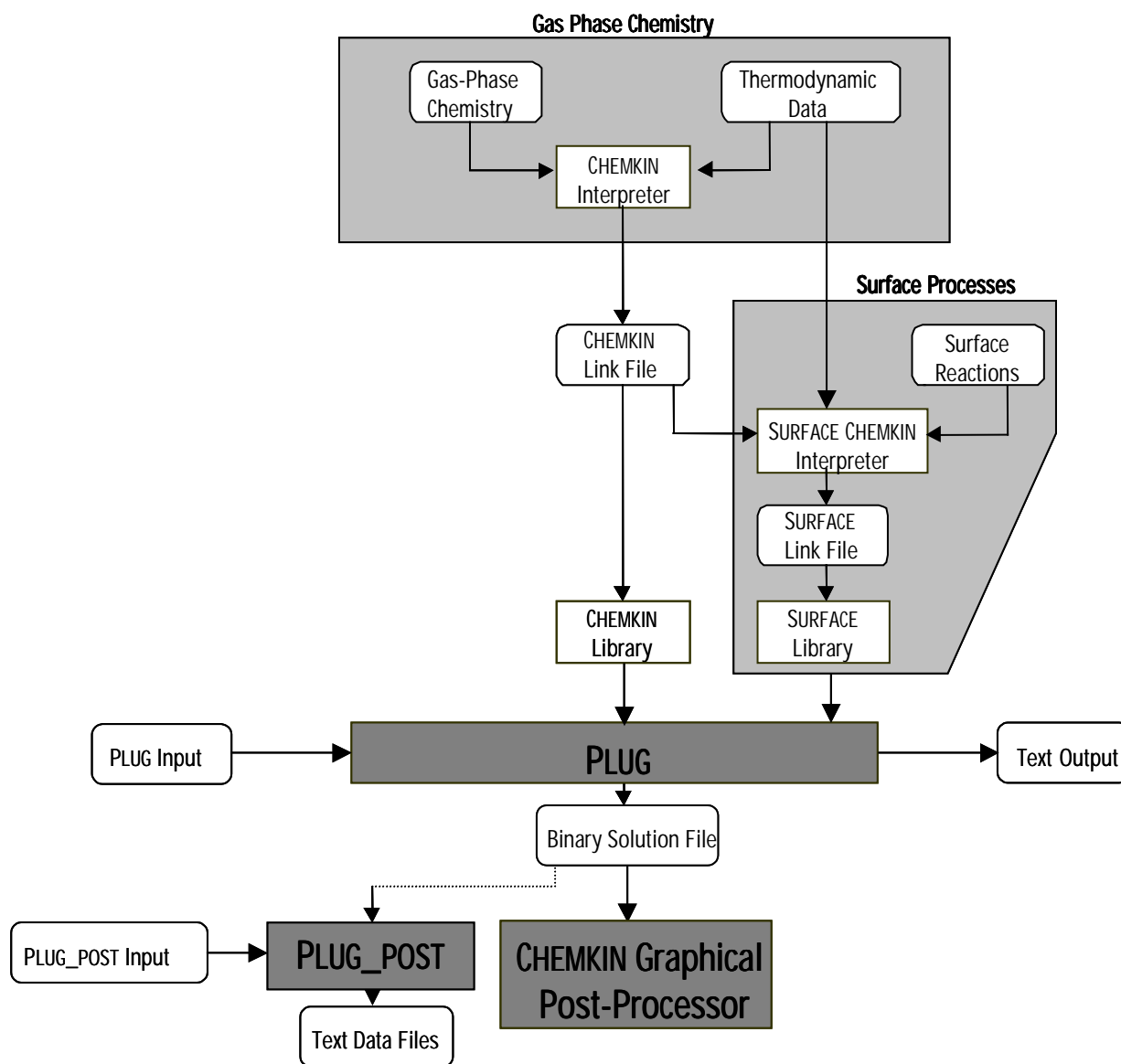
in conjunction with Eq. (7) until steady state is reached. Here  $\sigma_k$  is the site occupancy number for species  $k$  and  $\Gamma$  is the total site density of the phase in question. The initial values of  $Z_k$  for Eqs. (14) are essentially arbitrary (unless there are multiple steady states), although better guesses will naturally lead to faster convergence.

### 3. PROGRAM STRUCTURE

The CHEMKIN Application User Interface runs the PLUG program automatically through a mouse-driven interface and then allows the user to directly launch visualization of solution results using the CHEMKIN Graphical Post-processor. The PLUG program has a modular structure that interfaces to the CHEMKIN Utility package for obtaining kinetic, thermodynamic, and transport parameters. In addition to input directly from the user, PLUG depends on data obtained from the CHEMKIN Gas-phase and SURFACE CHEMKIN Utility packages. Therefore, to solve a reacting-flow problem the user must first execute the two preprocessor programs, “chem” and “surf”, which have access to the thermodynamic database (e.g. “therm.dat”). PLUG then reads input from the user (described in Chapter 4), defines the governing equations, solves the equations, and prints solutions for the reacting-flow problem. The CHEMKIN Graphical Post-processor can then be launched from the Application User Interface to plot solution data. Figure 1 shows the relationships between these components. For more information about the CHEMKIN Application User Interface or Graphical Post-processor, please see the CHEMKIN Getting Started manual.

The first step is to execute the CHEMKIN Interpreter, “chem”. The CHEMKIN Interpreter first reads user-supplied information about the species and chemical reactions for a particular reaction mechanism. It then extracts further information about the species’ thermodynamic properties from a database (e.g. “therm.dat”). The user may also optionally input thermodynamic property data directly in the input file to the CHEMKIN Interpreter to override or supplement the database information. The information from the user input and the thermodynamic properties is stored in the CHEMKIN Linking File, “chem.asc”; a file that is needed by the SURFACE CHEMKIN Interpreter, and later by the CHEMKIN subroutine library, which will be accessed by the PLUG program. The CHEMKIN Interpreter also writes text output (e.g. “chem.out”) that includes a formatted display of the user input and diagnostic messages from the Interpreter.

The SURFACE CHEMKIN Interpreter must next be executed after the CHEMKIN Interpreter has been run, because it relies on gas-phase species and element information in the CHEMKIN Linking file. The SURFACE CHEMKIN Interpreter reads user-supplied information (e.g., “surf.inp”) about surface and bulk species names, surface site types, surface reactions, and optional thermochemical information. This information is written to a SURFACE CHEMKIN Linking File (“surf.asc”), and later accessed by the SURFACE CHEMKIN subroutine library when called by the PLUG program. The SURFACE CHEMKIN Interpreter also generates a text file (e.g., “surf.out”) containing the input mechanism information and diagnostic messages.



**Figure 1. Relationship of PLUG to the CHEMKin and SURFACE CHEMKin pre-processors, and the associated input and output files.**

Once the pre-processors have run successfully, the PLUG program can then be executed. Since the CHEMKin and SURFACE CHEMKin subroutine libraries must be initialized before use, the PLUG program begins by making the appropriate initialization subroutine calls. The purpose of the initialization is to read the Linking Files and to set up the internal working and storage space required by all subroutines in the libraries.

PLUG then reads the user input that defines a particular reacting flow problem and the parameters needed to solve it. This input is read in Keyword format from the input file (e.g. “plug.inp”), described in Chapter 4. The program produces printed output (e.g. “plug.out”) and it saves the solution in a binary Save File, “save.bin”. The Save File can be read by the CHEMKIN Graphical Post-processor for plotting the solution results, as discussed further in Chapter 5.

### 3.1 Optional User Programming

In addition to using PLUG through the CHEMKIN Application User Interface, users have the flexibility to write their own interface to the reacting-flow model. To facilitate this, the PLUG program itself is written as a Fortran subroutine that may be called from a user-supplied driver routine. We provide examples of such driver routines as part of the PLUG software distribution, written in both C++ and Fortran. The driver routine performs the function of allocating total memory usage through definition of array sizes, as well as opening input and output files. PLUG checks internally to make sure that the allocated work arrays are sufficiently large to address the problem described by the input files. Programs can be linked to the PLUG subroutine by following the examples in the makefiles provided in the sample driver subdirectories (“drivers\_f77” or “drivers\_cpp”) of the standard distribution. Users taking advantage of this flexibility should be experienced with compiling and linking program files on their operating system and must have either a C++ or Fortran compiler installed.

In addition to the driver routine, the user can specify the reactor geometry with a user-written subroutine called GEOM. Similarly, the user can program the axial temperature profile with a function called TSPEC, and the external heat flux profile with a function called QE. Examples of these functions can be found in the CHEMKIN distribution, subdirectory “drivers\_cpp”, in a file named “plug\_user\_routines.f”. Before attempting to write these custom subroutines, the user should first consider the optional Keyword input described in Section 4.5, which provides the same flexibility but without the requirement of programming and re-compiling code.

### 3.2 The Save File

In addition to printed output, PLUG produces a binary solution file (“save.bin”) that contains the solution data. This file provides the ability to post-process the solution, using the CHEMKIN Graphical Post-processor or an alternative program. Further information on this subject will be found in the post-processing discussion in Chapter 5.

## 4. PROGRAM INPUT

### 4.1 Keyword Descriptions

Before running PLUG, the user must prepare three separate input files: one for CHEMKIN, one for SURFACE CHEMKIN, and one for PLUG itself. The first two are described in the respective user's manuals, so attention will be focused here on the third, which enables the user to specify the process parameters for a particular simulation. The file also contains some solution control options that should ideally have little effect on the final results, but which may allow the solution to be obtained more easily and/or accurately.

Each line in the input file begins with a keyword, which may be followed by a chemical species name and/or a numerical value. The specific rules governing keyword input are as follows:

1. The first four columns in the line are reserved for the keyword, which must begin in column 1.
2. Any other items on the line (species name and/or numerical value) can appear anywhere in columns 5-80.
3. A species name, if required, must appear before the corresponding numerical value and be separated from it by at least one space.
4. A species name must match exactly one of the names declared in the CHEMKIN or SURFACE CHEMKIN input file.
5. A numerical value can be stated in any format (integer, fixed point, or floating point). The precision (single vs. double) is determined by the program rather than by the input format.
6. If a keyword is repeated or conflicts with another, then the one last read takes precedence.
7. The last line must contain the keyword END alone. Aside from this, the order of the lines is unimportant.

A summary of the available keywords and their usage is given below. It should be emphasized that many of the keywords will not appear in a given input file, either because there are default values or because there are other (perhaps conflicting) options available. For each keyword, the short description indicates the circumstances, if any, under which it must be used.

## 4.2 Reactor Dimensions

**XSTR**— Inlet axial position.

Units: cm

Default value: 0.

Example: XSTR 1.5

**XEND**— Outlet axial position, equal to the overall reactor length if XSTR is zero.

Units: cm

Default value: None; this is required input.

Example: XEND 10.0

**DIAM**— Tube diameter. This is to be input only if the reactor is a round, empty tube of constant cross section (and with a negligible wall thickness if keyword QFIX or HEAT is used). Otherwise, the user-supplied subroutine GEOM must specify the reactor geometry, or keywords DPRO, AFLO, AINT, and/or AEXT can be used to describe the geometry.

Units: cm

Default value: None; if omitted, subroutine GEOM will be used.

Example: DIAM 5.3

## 4.3 Reactor Type

**ADIA**— Flag indicating that the reactor is adiabatic. This is the default.

Default: ADIA

**ISO**— Flag indicating that the reactor is isothermal, i.e., the temperature is constant at the value specified by TEMP.

Default: ADIA

**TFIX**— Flag indicating that the reactor has a user-specified axial temperature profile. In this case, the user may implement function TSPEC(X), which can be compiled with the driver routine for PLUG, or keyword TPRO to describe the profile. Any value specified with keyword TEMP would be ignored when TFIX is used.

Default: ADIA; a TSPEC function will not be used.

**QFIX**— Flag indicating that the reactor has a specified external heat flux profile. In this case, the user may implement function QE(X), which can be compiled with the driver routine for PLUG, or keyword QPRO to describe the profile.

Default: ADIA; a QE function will not be used.

**HEAT**— Flag indicating that the heat flux to the reactor will be calculated using a specified ambient temperature (TINF) and overall heat-transfer coefficient (BIGU).

Default: ADIA; zero heat loss.



## 4.4 Process Parameters

**TEMP**— Inlet gas temperature.

Units: Kelvins

Default value: None; this is required input unless keyword TFIX is used.

Example: TEMP 300.

**PRES**— Inlet pressure.

Units: atm

Default value: None; this is required input.

Example: PRES 1.0

**VEL**— Inlet velocity.

Units: cm/s

Default value: None; this is required input unless VDOT is specified.

Example: VEL 120.

**VDOT**— Inlet volumetric flow rate.

Units: cm<sup>3</sup>/s

Default value: None; this is required input unless VEL is specified.

Example: VDOT 100.

**MOLE** — Flag indicating that the input gas composition (keyword GAS) is in mole fractions. This is the default.

Default: MOLE

**MASS** — Flag indicating that the input gas composition (keyword GAS) is in mass fractions.

Default: MOLE

**GAS**— Inlet gas-phase mole or mass fraction (see keywords MOLE and MASS) for the given species. The input values will be normalized, but their sum must still be within 0.01 of unity.

Units: None

Default value: 0.

Example: GAS NH3 0.75

**VIS** — Viscosity of the inlet gas mixture.

Units: Poise (g/cm-s)

Default value: 0., i.e., viscous drag is neglected.

Example: VIS 0.01

**SURF**— Estimate (initial guess) for the inlet surface site fraction of the given species. The input values for each phase will be normalized, but their sum must still be within 0.01 of unity.

Units: None

Default value: 0.

Example: SURF HN\_SIF(S) 0.1

**BULK** — Bulk phase activity for the given species (assumed constant). The input values for each phase will be normalized, but their sum must still be within 0.01 of unity.

Units: None

Default value: 1.

Example: BULK SI(D) 1.0

**TINF** — Ambient temperature. This will be used only if keyword HEAT is specified.

Units: Kelvins

Default value: 298.

Example: TINF 300.

**BIGU** — Overall heat-transfer coefficient based on the internal surface area. This keyword will be ignored unless HEAT is specified.

Units:  $\text{erg}/\text{cm}^2\text{-s-K}$

Default value: None; this is required input if keyword HEAT is specified.

Example: BIGU 1.0E-3

## 4.5 Functional Variations with Distance

**DPRO** — Hydraulic diameter as a function of distance; input otherwise obtained from SUBROUTINE GEOM(X).

Units – cm, cm

Default – None.

Example: DPRO 0.0 1.0

**AFLO** — Cross-sectional area as a function of distance; input otherwise obtained from SUBROUTINE GEOM(X).

Units – cm,  $\text{cm}^2$

Default – None.

Example: AFLO 0.0 1.0

**AINT** — Deposition area per unit length; input otherwise obtained from SUBROUTINE GEOM(X).

Units – cm, cm

Default – None.

Example: AINT 0.0 1.0

**AEXT** — External surface area per unit length; input otherwise obtained from SUBROUTINE GEOM(X).

Units – cm, cm

Default – None.

Example: AEXT 0.0 1.0

(The following keywords pertain to the problem type specified by keyword TFIX only)

**TPRO**— Temperature as a function of distance; input otherwise obtained from SUBROUTINE TSPEC(X).

Units – cm, Kelvin

Default – None.

Example: TPRO 0.0 300.0

(The following keyword pertains to the problem type specified by keyword QFIX only)

**QPRO**— Heat flux as a function of distance; input otherwise obtained from SUBROUTINE QE(X).

Units – cm, erg/cm<sup>2</sup>/sec

Default – None.

Example: QPRO 0.0 0.0

## 4.6 Solution Control Parameters

**ATOL**— Absolute error tolerance used by DASSL.

Units: None

Default value: 10<sup>-8</sup>

Example: ATOL 1.0E-9

**RTOL**— Relative error tolerance used by DASSL.

Units: None

Default value: 10<sup>-6</sup>

Example: RTOL 1.0E-3

**DX**— Output distance interval. This governs the frequency of printing and has no effect on the accuracy of the solution.

Units: cm

Default value: 0.01

Example: DX 2.0

**NNEG** — Flag instructing DASSL to try to constrain all components of the solution vector to be non-negative. This is usually unnecessary, but it may help to use this keyword if negative solution components appear to be causing problems.

Default: Solution is not constrained.

**TSTP** — Initial time step for integration of the fictitious transient equations by DASSL. Steady state is assumed to be reached when there is no significant change in the surface site fractions over the course of one time step (see RCHG below). Clearly, this will be erroneous if the time step is simply too short to allow any significant reaction to take place. In this case the main reactor simulation should fail, with DASSL returning an error flag of IDID = -12. This signifies that DASSL is unable to adjust the initial derivatives so as to satisfy all of the equations at the reactor inlet, and this is a foregone conclusion if any purely algebraic equations are not already satisfied. Should this occur, the simulation should be repeated with a larger value for TSTP (or, perhaps, a smaller value for RCHG).

Units: sec

Default value: 1.

Example: TSTP 0.1

**RCHG** — Maximum relative change in the surface site fractions (over one time step) for which the fictitious transient equations can be considered to have converged to steady state. Caution: If this parameter is set too large relative to RTOL, then the main reactor simulation may fail with IDID = -12, as discussed above, because the algebraic equations will not appear to be satisfied at the inlet.

Units: None

Default value:  $10^{-6}$

Example: RCHG 1.0E-3

**ACHG** — Maximum absolute change in the surface site fractions (over one time step) for which the fictitious transient equations can be considered to have converged to steady state. The convergence test is made against the sum of the ACHG value plus the product of RCHG multiplied by the old site-fraction value. Therefore, if ACHG is set to zero (by default) then only RCHG is used to control the convergence criteria.

Units: None

Default value: 0

Example: ACHG 1.0E-7

**PSV** — Pseudo-velocity for use in modifying the surface species equations for improved convergence. This pseudo-convection term is incorporated into the surface site fraction equations in order to convert algebraic equations to differential equations. The value of the PSV should be small enough such that it has no effect on the solution results, but large enough to affect the convergence behavior. If not supplied, then the unmodified equations are used. The modified equations are sometimes helpful in reaching steady-state conditions for problems with stiff surface chemistry (e.g. catalytic combustion), but should not be used if no convergence problems are encountered. A recommended value to try for PSV would be about  $1/10^{\text{th}}$  of the inlet velocity, but the simulation should be repeated with smaller or larger values to make sure that it has no effect on the solution.

Units: cm/s

Default value: there is no pseudo convection velocity imposed at the surface.

Example: PSV 10.

**END—** Flag indicating the end of the input file. This line is required, and all subsequent lines will be ignored.

## 5. POST PROCESSING

### 5.1 CHEMKIN Graphical Post-processor

The CHEMKIN Graphical Post-processor provides a means for quick visualization of results from PLUG. Launched from the CHEMKIN Application User Interface, the Graphical Post-processor will automatically read in the solution data from the “save.bin” file in the working directory. Alternatively, the post-processor may be launched independently and a solution file may be opened from within the Post-processor. The user may open one or more solution files in the Post-processor and may also import external data for comparisons with the simulation results. In addition, the Graphical Post-processor can be used to export all of the solution data into comma-, tab-, or space-delimited text for further analysis with other software packages. For more information on the Graphical Post-processor, please see the CHEMKIN Getting Started manual.

### 5.2 Configurable Command-line Post-processor

In addition to the CHEMKIN Graphical Post-processor representation of solution data, we provide the user with a FORTRAN post-processor called PLUG\_POST. This program reads the binary solution file and prints selected data to text files, which can then be imported by many other graphics programs. The full source-code, `plug_post.f`, is provided in the CHEMKIN “post\_processors” subdirectory. Also in this directory is a makefile script for re-building the PLUG\_POST program, in case the user makes changes to the source code. In this way, the user may easily configure PLUG\_POST for his or her own analysis needs.

To run PLUG\_POST from the command-line, you will need to do the following:

1. Open a MS-DOS Prompt (PC) or shell (UNIX).
2. Change directories to your working directory, where your “save.bin” solution file resides.
3. Run PLUG\_POST from the command-line, specifying the full path to the CHEMKIN “bin” directory where the “plug\_post” executable resides, unless this is already in your environment “path” variable:

```
plug_post < plug_post.inp > plug_post.out
```

Here, “plug\_post.inp” is an input file that contains keywords described below. The output “plug\_post.out” will contain diagnostics and error messages for the PLUG\_POST run. PLUG\_POST will also create text files containing comma-separated values. The names for these files use a suffix (extension) of “.csv”.

PLUG\_POST uses keyword input. The available keywords are printed as a banner when the program is invoked; they are also described briefly here:

|             |   |
|-------------|---|
| <b>PREF</b> | Requests the text file name be prefixed by a character string.<br>Default – “plug”<br>Example: PREF plug  |
| <b>SPEC</b> | Requests species fractions for a space-delimited list of species, or “ALL”.<br>Default - none<br>Example: SPEC H2 O2 OH H2O HO2 H O               |
| <b>MOLE</b> | Print species as mole fractions.<br>Default - MOLE.   |
| <b>MASS</b> | Print species as mass fractions.<br>Default - MOLE.   |
| <b>SMIN</b> | Do not print species whose maximum fraction is less than SMIN.<br>Default – 0.0.  |
| <b>RATE</b> | Print chemical production rates for a space-delimited list of species, or “ALL”.<br>Default - No production rates printed.<br>Example: RATE OH NO |
| <b>DROP</b> | Eliminate reactions where relative (percent) chemical production rates are low.<br>Default – No filtering.<br>Example: DROP .20                   |
| <b>HELP</b> | Print a brief guide to keyword input.   |
| <b>END</b>  | Begin post-processing.  |

## 6. SAMPLE PROBLEM

This section contains the input and output files for a sample problem involving the chemical vapor deposition of silicon nitride ( $\text{Si}_3\text{N}_4$ ) from  $\text{SiF}_4$  and  $\text{NH}_3$ . Since the CHEMKIN and SURFACE CHEMKIN input and output files are described in their respective user's manuals, the following discussion will focus on the input and output specific to PLUG.

The input file specifies a process in which a gas mixture with an  $\text{NH}_3/\text{SiF}_4$  mole ratio of 6:1 is fed into a tubular reactor at a rate of 588 sccm. The inlet pressure is 2 Torr, and, because the surface kinetic data is valid only at 1713 K, the entire reactor is maintained at this temperature. The length and diameter of the reactor are 60 cm and 5.08 cm, respectively. From this information it can be shown that the axial Peclet number based on inlet conditions is about 70, while the radial Damkohler number is roughly 0.2. It follows that the plug flow assumptions are reasonably well satisfied by this process.

The input file also contains initial guesses for the surface site fractions at the reactor inlet. To demonstrate the ability of PLUG to obtain a solution with a bad initial guess, these are assigned the same value of 1/6.

PLUG is able to solve this problem with no apparent difficulty, and the output file shown below contains the results. First, the version numbers for PLUG, CHEMKIN, and SURFACE CHEMKIN are printed. Echoing of the keyword input follows. If any errors are detected in the PLUG input file, appropriate messages would be printed here. Next is a statement that PLUG was successful in integrating the transient equations to steady state, (despite the poor quality of the initial estimates). This yields the true surface site fractions at the inlet and allows the main reactor simulation to begin.

The results of the computation are printed at intervals of 10 cm, as specified by the keyword DX. At each point there is information about the states of the gas and surface phases, the gas flow velocity, the residence time, and the bulk-phase deposition rates. Several interesting features can be noted. First, it is clear that there is very little gas-phase reaction occurring: at the reactor exit, 99.99% of the gas is comprised of  $\text{SiF}_4$ ,  $\text{NH}_3$ , and HF. On the other hand, the surface processes are fairly rapid, causing  $\text{SiF}_4$  to be severely depleted and HF to build up. The resultant net increase in the number of gas-phase molecules causes the flow velocity to rise by 17% between the inlet and the exit. Still, the overall pressure drop is a barely perceptible 0.04 Torr.

Turning to the solid phases, one sees that the surface is dominated by the species  $\text{HN\_NH}_2(\text{S})$ ; not surprisingly, the same result has been observed in other reactor simulations. Of more practical interest is the  $\text{Si}_3\text{N}_4$  deposition rate, which falls by a factor of 3 along the reactor. This is a direct result of the  $\text{SiF}_4$  depletion noted above. At all points, however, the Si:N molar deposition ratio is maintained precisely at 0.75.



## 6.1 CHEMKIN Input File for Sample Problem

```
ELEMENTS H N SI F
END
SPECIES
H2 H N2 N NH NH2 NNH N2H2 N2H3 N2H4
HF F SIF4 SIF3 SIHF3 SIF3NH2
NH3
END
THERMO
SI          J 3/67SI  100 0000 0000 00G   300.000  5000.000          1
  0.26506014E 01-0.35763852E-03 0.29592293E-06-0.72804829E-10 0.57963329E-14  2
  0.53437054E 05 0.52204057E 01 0.31793537E 01-0.27646992E-02 0.44784038E-05  3
-0.32833177E-08 0.91213631E-12 0.53339032E 05 0.27273204E 01          4
SIF2        41889SI  1F   2   0   0G   300.000  3000.000 1000.00    0 1
  0.61424704E+01 0.78079745E-03-0.13393120E-06-0.62648393E-10 0.17251383E-13  2
-0.77440422E+05-0.47123275E+01 0.38453453E+01 0.60384651E-02-0.11677322E-05  3
-0.45795536E-08 0.26074143E-11-0.76816336E+05 0.72729836E+01          4
SIF         41889SI  1F   1   0   0G   300.000  3000.000 1000.00    0 1
  0.41200666E+01 0.35488207E-03-0.72002223E-07-0.21904345E-10 0.67645906E-14  2
-0.75613784E+04 0.27842460E+01 0.31449478E+01 0.25885573E-02-0.57959124E-06  3
-0.18072788E-08 0.10411718E-11-0.72944390E+04 0.78767738E+01          4
SIF3NH2     41889SI  1N   1F   3H   2G   300.000  3000.000 1000.00    0 1
  0.12109636E+02 0.43832823E-02-0.41422453E-06-0.39890902E-09 0.89589543E-13  2
-0.16417678E+06-0.30469284E+02 0.62294030E+01 0.17780151E-01-0.26123043E-05  3
-0.12672435E-07 0.70445559E-11-0.16258489E+06 0.20454407E+00          4
SIHF3       41889SI  1H   1F   3   0G   300.000  3000.000 1000.00    0 1
  0.93635674E+01 0.29475559E-02-0.35776330E-06-0.28582245E-09 0.69157286E-13  2
-0.14860736E+06-0.21694529E+02 0.39180529E+01 0.14639172E-01-0.18560698E-05  3
-0.10582003E-07 0.56175433E-11-0.14704386E+06 0.70242615E+01          4
SIF3        41889SI  1F   3   0   0G   300.000  3000.000 1000.00    0 1
  0.85247898E+01 0.13237924E-02-0.21042787E-06-0.11495040E-09 0.30553014E-13  2
-0.12235223E+06-0.15502343E+02 0.46628685E+01 0.10087878E-01-0.18055442E-05  3
-0.77692990E-08 0.43778518E-11-0.12129652E+06 0.46729660E+01          4
SIF4        J 6/76SI  1F   4   0   0G   300.000  5000.000          1
  0.10478473E 02 0.28586756E-02-0.12646314E-05 0.24746863E-09-0.17824296E-13  2
-0.19790550E 06-0.27520641E 02 0.21893068E 01 0.33702007E-01-0.46723179E-04  3
  0.31584638E-07-0.84506114E-11-0.19603289E 06 0.13287308E 02          4
HF          J 6/77H   1F   1   0   0G   300.000  5000.000          1
  0.29919110E 01 0.71489475E-03-0.68630973E-07-0.11617130E-10 0.19412375E-14  2
-0.33621364E 05 0.38123288E 01 0.34379986E 01 0.53571598E-03-0.15229655E-05  3
  0.17564491E-08-0.57869940E-12-0.33818972E 05 0.11930153E 01          4
F          J 9/65F   1   0   0   0G   300.000  5000.000          1
  0.27004353E 01-0.22293182E-03 0.97941385E-07-0.19123038E-10 0.13768154E-14  2
  0.87163617E 04 0.38067182E 01 0.28128740E 01-0.33023098E-05-0.12897310E-05  3
  0.16837365E-08-0.64587833E-12 0.86604019E 04 0.30984198E 01          4
END
```

|                    |           |        |           |              |
|--------------------|-----------|--------|-----------|--------------|
| REACTIONS          |           |        |           |              |
| H+H+M=H2+M         | 0.100E+19 | -1.000 | 0.000     | ! D-L        |
| H2/0.0/            |           |        |           |              |
| H+H+H2=H2+H2       | 0.920E+17 | -0.600 | 0.000     |              |
| NH+N=N2+H          | 0.300E+14 | 0.000  | 0.000     | ! JAM        |
| NH+H=N+H2          | 0.100E+15 | 0.000  | 0.000     | ! NH3 CST    |
| NH2+H=NH+H2        | 0.692E+14 | 0.000  | 3650.000  |              |
| NH3+H=NH2+H2       | 0.636E+06 | 2.390  | 10171.000 | ! MICHAEL    |
| NNH=N2+H           | 0.100E+05 | 0.000  | 0.000     | ! JAM        |
| NNH+H=N2+H2        | 0.100E+15 | 0.000  | 0.000     | ! JAM        |
| NNH+NH2=N2+NH3     | 0.500E+14 | 0.000  | 0.000     | ! JAM        |
| NNH+NH=N2+NH2      | 0.500E+14 | 0.000  | 0.000     | ! JAM        |
| NH2+NH=N2H2+H      | 0.500E+14 | 0.000  | 0.000     | ! NH3CST     |
| NH+NH=N2+H+H       | 0.254E+14 | 0.000  | 0.000     | ! NH3 CST    |
| NH2+N=N2+H+H       | 0.720E+14 | 0.000  | 0.000     | ! PG         |
| N2H2+M=NNH+H+M     | 0.500E+17 | 0.000  | 50000.000 | ! NH3 CST    |
| N2/2/ H2/2/        |           |        |           |              |
| N2H2+H=NNH+H2      | 0.500E+14 | 0.000  | 1000.000  | ! NH3 CST    |
| N2H2+NH=NNH+NH2    | 0.100E+14 | 0.000  | 1000.000  | ! NH3 CST    |
| N2H2+NH2=NH3+NNH   | 0.100E+14 | 0.000  | 1000.000  | ! NH3 CST    |
| NH2+NH2=N2H2+H2    | 0.500E+12 | 0.000  | 0.000     | ! NH3 CST    |
| NH3+M=NH2+H+M      | 0.140E+17 | 0.000  | 90600.000 | ! MSGK       |
| N2H3+H=NH2+NH2     | 1.60E+12  | 0.0    | 0.0       | ! MSGK       |
| N2H3+M=N2H2+H+M    | 3.50E+16  | 0.0    | 46000.0   | ! MSGK       |
| N2H3+NH=NH2+N2H2   | 2.00E+13  | 0.0    | 0.0       | ! MSGK       |
| NH2+NH2+M=N2H4+M   | 3.00E+20  | -1.0   | 0.0       | ! MSGK       |
| H+N2H4=H2+N2H3     | 1.30E+13  | 0.0    | 2500.0    | ! MSGK       |
| NH2+N2H4=NH3+N2H3  | 3.90E+12  | 0.0    | 1500.0    | ! MSGK       |
| NH+H+M=NH2+M       | 2.00E+16  | -0.5   | 0.0       | ! MSGK       |
| NH2+NH2=NH3+NH     | 5.00E+12  | 0.0    | 10000.0   | ! MSGK       |
| F+NH3=NH2+HF       | 4.27E+11  | 0.5    | 800.0     | ! KONDRATIEV |
| SIF4=SIF3+F        | 3.00E+12  | 0.0    | 147170.0  | ! PHO&MEC    |
| H+SIF4=HF+SIF3     | 1.00E+13  | 0.0    | 50000.0   | ! PHO&MEC    |
| NH2+SIF4=SIF3NH2+F | 1.00E+11  | 0.0    | 40950.0   | ! GUESS      |
| NH3+SIF3=SIF3NH2+H | 1.00E+11  | 0.0    | 5000.0    | ! GUESS      |
| NH3+SIF3=SIHF3+NH2 | 1.00E+11  | 0.0    | 10000.0   | ! PHO&MEC    |
| END                |           |        |           |              |

## 6.2 CHEMKIN Output File for Sample Problem

CHEMKIN-III GAS-PHASE MECHANISM INTERPRETER:  
 DOUBLE PRECISION Vers. 6.24 2000/06/18  
 Copyright 1995, Sandia Corporation.  
 The U.S. Government retains a limited license in this software.

|             |  | ELEMENTS<br>CONSIDERED |    | ATOMIC<br>WEIGHT |             |               |   |   |    |   |
|-------------|--|------------------------|----|------------------|-------------|---------------|---|---|----|---|
|             |  | 1.                     | H  | 1.00797          |             |               |   |   |    |   |
|             |  | 2.                     | N  | 14.0067          |             |               |   |   |    |   |
|             |  | 3.                     | SI | 28.0860          |             |               |   |   |    |   |
|             |  | 4.                     | F  | 18.9984          |             |               |   |   |    |   |
|             |  |                        |    |                  |             |               |   |   |    |   |
|             |  | C                      |    |                  |             |               |   |   |    |   |
|             |  | P H                    |    |                  |             |               |   |   |    |   |
|             |  | H A                    |    |                  |             |               |   |   |    |   |
|             |  | A R                    |    |                  |             |               |   |   |    |   |
|             |  | S G                    |    |                  |             |               |   |   |    |   |
| SPECIES     |  |                        |    | MOLECULAR        | TEMPERATURE | ELEMENT COUNT |   |   |    |   |
| CONSIDERED  |  | E                      | E  | WEIGHT           | LOW         | HIGH          | H | N | SI | F |
|             |  |                        |    |                  |             |               |   |   |    |   |
| 1. H2       |  | G                      | 0  | 2.01594          | 300         | 5000          | 2 | 0 | 0  | 0 |
| 2. H        |  | G                      | 0  | 1.00797          | 300         | 5000          | 1 | 0 | 0  | 0 |
| 3. N2       |  | G                      | 0  | 28.01340         | 300         | 5000          | 0 | 2 | 0  | 0 |
| 4. N        |  | G                      | 0  | 14.00670         | 300         | 5000          | 0 | 1 | 0  | 0 |
| 5. NH       |  | G                      | 0  | 15.01467         | 300         | 5000          | 1 | 1 | 0  | 0 |
| 6. NH2      |  | G                      | 0  | 16.02264         | 300         | 5000          | 2 | 1 | 0  | 0 |
| 7. NNH      |  | G                      | 0  | 29.02137         | 250         | 4000          | 1 | 2 | 0  | 0 |
| 8. N2H2     |  | G                      | 0  | 30.02934         | 300         | 5000          | 2 | 2 | 0  | 0 |
| 9. N2H3     |  | G                      | 0  | 31.03731         | 300         | 5000          | 3 | 2 | 0  | 0 |
| 10. N2H4    |  | G                      | 0  | 32.04528         | 300         | 5000          | 4 | 2 | 0  | 0 |
| 11. HF      |  | G                      | 0  | 20.00637         | 300         | 5000          | 1 | 0 | 0  | 1 |
| 12. F       |  | G                      | 0  | 18.99840         | 300         | 5000          | 0 | 0 | 0  | 1 |
| 13. SIF4    |  | G                      | 0  | 104.07960        | 300         | 5000          | 0 | 0 | 1  | 4 |
| 14. SIF3    |  | G                      | 0  | 85.08120         | 300         | 3000          | 0 | 0 | 1  | 3 |
| 15. SIHF3   |  | G                      | 0  | 86.08917         | 300         | 3000          | 1 | 0 | 1  | 3 |
| 16. SIF3NH2 |  | G                      | 0  | 101.10384        | 300         | 3000          | 2 | 1 | 1  | 3 |
| 17. NH3     |  | G                      | 0  | 17.03061         | 300         | 5000          | 3 | 1 | 0  | 0 |

| REACTIONS CONSIDERED |             |           |  | (k = A T**b exp(-E/RT)) |      |         |
|----------------------|-------------|-----------|--|-------------------------|------|---------|
|                      |             |           |  | A                       | b    | E       |
| 1. H+H+M=H2+M        |             |           |  | 1.00E+18                | -1.0 | 0.0     |
| H2                   | Enhanced by | 0.000E+00 |  |                         |      |         |
| 2. H+H+H2=H2+H2      |             |           |  | 9.20E+16                | -0.6 | 0.0     |
| 3. NH+N=N2+H         |             |           |  | 3.00E+13                | 0.0  | 0.0     |
| 4. NH+H=N+H2         |             |           |  | 1.00E+14                | 0.0  | 0.0     |
| 5. NH2+H=NH+H2       |             |           |  | 6.92E+13                | 0.0  | 3650.0  |
| 6. NH3+H=NH2+H2      |             |           |  | 6.36E+05                | 2.4  | 10171.0 |
| 7. NNH=N2+H          |             |           |  | 1.00E+04                | 0.0  | 0.0     |
| 8. NNH+H=N2+H2       |             |           |  | 1.00E+14                | 0.0  | 0.0     |
| 9. NNH+NH2=N2+NH3    |             |           |  | 5.00E+13                | 0.0  | 0.0     |
| 10. NNH+NH=N2+NH2    |             |           |  | 5.00E+13                | 0.0  | 0.0     |
| 11. NH2+NH=N2H2+H    |             |           |  | 5.00E+13                | 0.0  | 0.0     |
| 12. NH+NH=N2+H+H     |             |           |  | 2.54E+13                | 0.0  | 0.0     |
| 13. NH2+N=N2+H+H     |             |           |  | 7.20E+13                | 0.0  | 0.0     |
| 14. N2H2+M=NNH+H+M   |             |           |  | 5.00E+16                | 0.0  | 50000.0 |
| N2                   | Enhanced by | 2.000E+00 |  |                         |      |         |
| H2                   | Enhanced by | 2.000E+00 |  |                         |      |         |
| 15. N2H2+H=NNH+H2    |             |           |  | 5.00E+13                | 0.0  | 1000.0  |
| 16. N2H2+NH=NNH+NH2  |             |           |  | 1.00E+13                | 0.0  | 1000.0  |
| 17. N2H2+NH2=NH3+NNH |             |           |  | 1.00E+13                | 0.0  | 1000.0  |
| 18. NH2+NH2=N2H2+H2  |             |           |  | 5.00E+11                | 0.0  | 0.0     |
| 19. NH3+M=NH2+H+M    |             |           |  | 1.40E+16                | 0.0  | 90600.0 |

|  |          |      |          |
|--|----------|------|----------|
| 20. $\text{N}_2\text{H}_3 + \text{H} = \text{NH}_2 + \text{NH}_2$                  | 1.60E+12 | 0.0  | 0.0      |
| 21. $\text{N}_2\text{H}_3 + \text{M} = \text{N}_2\text{H}_2 + \text{H} + \text{M}$ | 3.50E+16 | 0.0  | 46000.0  |
| 22. $\text{N}_2\text{H}_3 + \text{NH} = \text{NH}_2 + \text{N}_2\text{H}_2$        | 2.00E+13 | 0.0  | 0.0      |
| 23. $\text{NH}_2 + \text{NH}_2 + \text{M} = \text{N}_2\text{H}_4 + \text{M}$       | 3.00E+20 | -1.0 | 0.0      |
| 24. $\text{H} + \text{N}_2\text{H}_4 = \text{H}_2 + \text{N}_2\text{H}_3$          | 1.30E+13 | 0.0  | 2500.0   |
| 25. $\text{NH}_2 + \text{N}_2\text{H}_4 = \text{NH}_3 + \text{N}_2\text{H}_3$      | 3.90E+12 | 0.0  | 1500.0   |
| 26. $\text{NH} + \text{H} + \text{M} = \text{NH}_2 + \text{M}$                     | 2.00E+16 | -0.5 | 0.0      |
| 27. $\text{NH}_2 + \text{NH}_2 = \text{NH}_3 + \text{NH}$                          | 5.00E+12 | 0.0  | 10000.0  |
| 28. $\text{F} + \text{NH}_3 = \text{NH}_2 + \text{HF}$                             | 4.27E+11 | 0.5  | 800.0    |
| 29. $\text{SiF}_4 = \text{SiF}_3 + \text{F}$                                       | 3.00E+12 | 0.0  | 147170.0 |
| 30. $\text{H} + \text{SiF}_4 = \text{HF} + \text{SiF}_3$                           | 1.00E+13 | 0.0  | 50000.0  |
| 31. $\text{NH}_2 + \text{SiF}_4 = \text{SiF}_3\text{NH}_2 + \text{F}$              | 1.00E+11 | 0.0  | 40950.0  |
| 32. $\text{NH}_3 + \text{SiF}_3 = \text{SiF}_3\text{NH}_2 + \text{H}$              | 1.00E+11 | 0.0  | 5000.0   |
| 33. $\text{NH}_3 + \text{SiF}_3 = \text{SiHF}_3 + \text{NH}_2$                     | 1.00E+11 | 0.0  | 10000.0  |

NOTE: A units mole-cm-sec-K, E units cal/mole

NO ERRORS FOUND ON INPUT:  
ASCII Vers. 1.1 CHEMKIN linkfile chem.asc written.

WORKING SPACE REQUIREMENTS ARE  
 INTEGER: 1086  
 REAL: 723  
 CHARACTER: 21  
 Total CPUtime (sec): 0.15625

### 6.3 SURFACE CHEMKIN Input File for Sample Problem

```

SITE/SI3N4/      SDEN/4.1683E-9/
  HN_SIF(S)/2/  F3SI_NH2(S)/2/  F2SINH(S)/2/
  H2NFSINH(S)/2/  HN(FSINH)2(S)/4/
  HN_NH2(S)/2/
END
BULK SI(D)/2.066/
BULK N(D) /1.374/
END
THERMO ALL
  300.      600.      1685.
HN_SIF(S)      J 3/67N  1H  1SI  1F  1S  300.000  1685.000      1
  0.24753989E 01 0.88112187E-03-0.20939481E-06 0.42757187E-11 0.16006564E-13      2
-0.81255620E 03-0.12188747E 02 0.84197538E 00 0.83710416E-02-0.13077030E-04      3
  0.97593603E-08-0.27279380E-11-0.52486288E 03-0.45272678E 01      4
HN_NH2(S)      J 3/67N  2H  3SI  0F  0S  300.000  1685.000      1
  0.24753989E 01 0.88112187E-03-0.20939481E-06 0.42757187E-11 0.16006564E-13      2
-0.81255620E 03-0.12188747E 02 0.84197538E 00 0.83710416E-02-0.13077030E-04      3
  0.97593603E-08-0.27279380E-11-0.52486288E 03-0.45272678E 01      4
F3SI_NH2(S)    J 3/67N  1H  2SI  1F  3S  300.000  1685.000      1
  0.24753989E 01 0.88112187E-03-0.20939481E-06 0.42757187E-11 0.16006564E-13      2
-0.81255620E 03-0.12188747E 02 0.84197538E 00 0.83710416E-02-0.13077030E-04      3
  0.97593603E-08-0.27279380E-11-0.52486288E 03-0.45272678E 01      4
F2SINH(S)      J 3/67N  1H  1SI  1F  2S  300.000  1685.000      1
  0.24753989E 01 0.88112187E-03-0.20939481E-06 0.42757187E-11 0.16006564E-13      2
-0.81255620E 03-0.12188747E 02 0.84197538E 00 0.83710416E-02-0.13077030E-04      3
  0.97593603E-08-0.27279380E-11-0.52486288E 03-0.45272678E 01      4
H2NFSINH(S)    J 3/67N  2H  3SI  1F  1S  300.000  1685.000      1
  0.24753989E 01 0.88112187E-03-0.20939481E-06 0.42757187E-11 0.16006564E-13      2
-0.81255620E 03-0.12188747E 02 0.84197538E 00 0.83710416E-02-0.13077030E-04      3
  0.97593603E-08-0.27279380E-11-0.52486288E 03-0.45272678E 01      4
HN(FSINH)2(S)  J 3/67N  3H  3SI  2F  2S  300.000  1685.000      1
  0.24753989E 01 0.88112187E-03-0.20939481E-06 0.42757187E-11 0.16006564E-13      2
-0.81255620E 03-0.12188747E 02 0.84197538E 00 0.83710416E-02-0.13077030E-04      3
  0.97593603E-08-0.27279380E-11-0.52486288E 03-0.45272678E 01      4
SI(D)          J 3/67SI  100 000 000 0S  300.000  1685.000      1
  0.24753989E 01 0.88112187E-03-0.20939481E-06 0.42757187E-11 0.16006564E-13      2
-0.81255620E 03-0.12188747E 02 0.84197538E 00 0.83710416E-02-0.13077030E-04      3
  0.97593603E-08-0.27279380E-11-0.52486288E 03-0.45272678E 01      4
N(D)          J 3/67N  100 000 000 0S  300.000  1685.000      1
  0.24753989E 01 0.88112187E-03-0.20939481E-06 0.42757187E-11 0.16006564E-13      2
-0.81255620E 03-0.12188747E 02 0.84197538E 00 0.83710416E-02-0.13077030E-04      3
  0.97593603E-08-0.27279380E-11-0.52486288E 03-0.45272678E 01      4
END
REACTIONS
  NH3          + HN_SIF(S) => HN_NH2(S)  + SI(D) + HF      7.562E08  0.5 0.0
  SIF4         + HN_NH2(S) => F3SI_NH2(S) + N(D)  + HF      3.0967E8  0.5 0.0
  F3SI_NH2(S)          => F2SINH(S)      + HF      1.0E05  0.0 0.0
  NH3          + F2SINH(S) => H2NFSINH(S)      + HF      7.562E08  0.5 0.0
  H2NFSINH(S)  + F2SINH(S) => HN(FSINH)2(S)      + HF      1.0E15  0.0 0.0
  HN(FSINH)2(S) + F2SINH(S) => 3HN_SIF(S) + N(D) + HF      1.0E15  0.0 0.0
END

```

## 6.4 SURFACE CHEMKIN Output File for Sample Problem

CHEMKIN-III SURFACE MECHANISM INTERPRETER:  
DOUBLE PRECISION Vers. 7.20 2000/06/18  
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CKLIB: CHEMKIN-III GAS-PHASE CHEMICAL KINETICS LIBRARY,  
DOUBLE PRECISION Vers. 5.28 2000/08/05  
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| SPECIES    | MOLECULAR |         |        | ELEMENT COUNT |
|------------|-----------|---------|--------|---------------|
| CONSIDERED | WEIGHT    | Density | Nsites | H N SI F      |

Gas phase species:

|             |           |  |  |   |   |   |   |
|-------------|-----------|--|--|---|---|---|---|
| 1. H2       | 2.01594   |  |  | 2 | 0 | 0 | 0 |
| 2. H        | 1.00797   |  |  | 1 | 0 | 0 | 0 |
| 3. N2       | 28.01340  |  |  | 0 | 2 | 0 | 0 |
| 4. N        | 14.00670  |  |  | 0 | 1 | 0 | 0 |
| 5. NH       | 15.01467  |  |  | 1 | 1 | 0 | 0 |
| 6. NH2      | 16.02264  |  |  | 2 | 1 | 0 | 0 |
| 7. NNH      | 29.02137  |  |  | 1 | 2 | 0 | 0 |
| 8. N2H2     | 30.02934  |  |  | 2 | 2 | 0 | 0 |
| 9. N2H3     | 31.03731  |  |  | 3 | 2 | 0 | 0 |
| 10. N2H4    | 32.04528  |  |  | 4 | 2 | 0 | 0 |
| 11. HF      | 20.00637  |  |  | 1 | 0 | 0 | 1 |
| 12. F       | 18.99840  |  |  | 0 | 0 | 0 | 1 |
| 13. SIF4    | 104.07960 |  |  | 0 | 0 | 1 | 4 |
| 14. SIF3    | 85.08120  |  |  | 0 | 0 | 1 | 3 |
| 15. SIHF3   | 86.08917  |  |  | 1 | 0 | 1 | 3 |
| 16. SIF3NH2 | 101.10384 |  |  | 2 | 1 | 1 | 3 |
| 17. NH3     | 17.03061  |  |  | 3 | 1 | 0 | 0 |

SITE: SI3N4 0.417E-08 moles/cm\*\*2

|                   |           |  |   |   |   |   |   |
|-------------------|-----------|--|---|---|---|---|---|
| 18. HN_SIF(S)     | 62.09907  |  | 2 | 1 | 1 | 1 | 1 |
| 19. F3SI_NH2(S)   | 101.10384 |  | 2 | 2 | 1 | 1 | 3 |
| 20. F2SINH(S)     | 81.09747  |  | 2 | 1 | 1 | 1 | 2 |
| 21. H2NFSINH(S)   | 78.12171  |  | 2 | 3 | 2 | 1 | 1 |
| 22. HN(FSINH)2(S) | 139.21281 |  | 4 | 3 | 3 | 2 | 2 |
| 23. HN_NH2(S)     | 31.03731  |  | 2 | 3 | 2 | 0 | 0 |

BULK: BULK1

|           |          |                   |  |   |   |   |   |
|-----------|----------|-------------------|--|---|---|---|---|
| 24. SI(D) | 28.08600 | 0.207E+01 g/cm**3 |  | 0 | 0 | 1 | 0 |
|-----------|----------|-------------------|--|---|---|---|---|

BULK: BULK2

|          |          |                   |  |   |   |   |   |
|----------|----------|-------------------|--|---|---|---|---|
| 25. N(D) | 14.00670 | 0.137E+01 g/cm**3 |  | 0 | 1 | 0 | 0 |
|----------|----------|-------------------|--|---|---|---|---|

| SURFACE REACTIONS CONSIDERED                       | (k = A T**b exp(-E/RT)) |     |     |
|--|-------------------------|-----|-----|
|  | A                       | b   | E   |
| 1. NH3+HN_SIF(S)=>HN_NH2(S)+SI(D)+HF               | 7.56E+08                | 0.5 | 0.0 |
| 2. SIF4+HN_NH2(S)=>F3SI_NH2(S)+N(D)+HF             | 3.10E+08                | 0.5 | 0.0 |
| 3. F3SI_NH2(S)=>F2SINH(S)+HF                       | 1.00E+05                | 0.0 | 0.0 |
| 4. NH3+F2SINH(S)=>H2NFSINH(S)+HF                   | 7.56E+08                | 0.5 | 0.0 |
| 5. H2NFSINH(S)+F2SINH(S)<br>=>HN(FSINH)2(S)+HF     | 1.00E+15                | 0.0 | 0.0 |
| 6. HN(FSINH)2(S)+F2SINH(S)<br>=>3HN_SIF(S)+N(D)+HF | 1.00E+15                | 0.0 | 0.0 |

NOTE: A units mole-cm-sec-K, E units cal/mole

NO ERRORS FOUND ON INPUT:

ASCII Version 1.1 surface linkfile surf.asc written.

WORKING SPACE REQUIREMENTS ARE

INTEGER: 481

REAL: 642

CHARACTER: 34

Total CPUtime (sec): 0.046875

## 6.5 PLUG Input File for Sample Problem

```
XEND          60.
DIAM          5.08
ISO
TEMP         1713.
PRES         2.632E-3
VDOT         23370.
GAS   SIF4    0.1427
GAS   NH3     0.8573
VIS          5.7E-4
SURF   HN_SIF(S)  0.1667
SURF   F3SI_NH2(S) 0.1667
SURF   F2SINH(S)  0.1666
SURF   H2NFSINH(S) 0.1666
SURF   HN(FSINH)2(S) 0.1667
SURF   HN_NH2(S)  0.1667
DX          10.
END
```



## 6.6 PLUG Output File for Sample Problem

PLUG: Plug Flow Reactor Code  
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there is a non-exclusive license for use of  
this work by or on behalf of  
the U. S. Government.  
Version 3.9, 2000/08/03  
DOUBLE PRECISION

|           | WORKING SPACE REQUIREMENTS<br>PROVIDED | REQUIRED |
|-----------|--|----------|
| INTEGER   | 1682                                   | 1682     |
| REAL      | 2833                                   | 2833     |
| CHARACTER | 59                                     | 59       |

CKLIB: CHEMKIN-III GAS-PHASE CHEMICAL KINETICS LIBRARY,  
DOUBLE PRECISION Vers. 5.28 2000/08/05  
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SKLIB: CHEMKIN-III SURFACE KINETICS LIBRARY,  
DOUBLE PRECISION Vers. 7.17 2000/07/02  
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|      |               |          |
|------|---------------|----------|
| XEND |               | 60.      |
| DIAM |               | 5.08     |
| ISO  |               |          |
| TEMP |               | 1713.    |
| PRES |               | 2.632E-3 |
| VDOT |               | 23370.   |
| GAS  | SIF4          | 0.1427   |
| GAS  | NH3           | 0.8573   |
| VIS  |               | 5.7E-4   |
| SURF | HN_SIF(S)     | 0.1667   |
| SURF | F3SI_NH2(S)   | 0.1667   |
| SURF | F2SINH(S)     | 0.1666   |
| SURF | H2NFSINH(S)   | 0.1666   |
| SURF | HN(FSINH)2(S) | 0.1667   |
| SURF | HN_NH2(S)     | 0.1667   |
| DX   |               | 10.      |
| END  |               |          |

SITE FRACTIONS AT REACTOR INLET FOUND SUCCESSFULLY

X = 0.000E+00 CM  
 RESIDENCE TIME = 0.000E+00 S  
 TEMPERATURE = 1713.0 K  
 GAS DENSITY = 5.515E-07 G/CM\*\*3  
 PRESSURE = 2.000E+00 TORR  
 VELOCITY = 1.153E+03 CM/S  
 TOTAL DEPOSITION RATE = 3.056E-06 G/CM\*\*2/S  
 GAS-PHASE MOLE FRACTIONS  

|         |             |      |             |       |             |
|---------|-------------|------|-------------|-------|-------------|
| H2      | = 0.000E+00 | H    | = 0.000E+00 | N2    | = 0.000E+00 |
| N       | = 0.000E+00 | NH   | = 0.000E+00 | NH2   | = 0.000E+00 |
| NNH     | = 0.000E+00 | N2H2 | = 0.000E+00 | N2H3  | = 0.000E+00 |
| N2H4    | = 0.000E+00 | HF   | = 0.000E+00 | F     | = 0.000E+00 |
| SIF4    | = 1.427E-01 | SIF3 | = 0.000E+00 | SIHF3 | = 0.000E+00 |
| SIF3NH2 | = 0.000E+00 | NH3  | = 8.573E-01 |       |             |

 SURFACE SITE FRACTIONS  

|             |             |               |             |           |             |
|-------------|-------------|---------------|-------------|-----------|-------------|
| HN_SIF(S)   | = 6.242E-02 | F3SI_NH2(S)   | = 3.136E-04 | F2SINH(S) | = 2.081E-02 |
| H2NFSINH(S) | = 2.411E-04 | HN(FSINH)2(S) | = 4.821E-04 | HN_NH2(S) | = 9.157E-01 |

 BULK SPECIES DEPOSITION RATES (MOL/CM\*\*2/S)  

|       |             |      |             |
|-------|-------------|------|-------------|
| SI(D) | = 6.536E-08 | N(D) | = 8.715E-08 |
|-------|-------------|------|-------------|

  
 X = 1.000E+01 CM  
 RESIDENCE TIME = 8.502E-03 S  
 TEMPERATURE = 1713.0 K  
 GAS DENSITY = 5.124E-07 G/CM\*\*3  
 PRESSURE = 1.994E+00 TORR  
 VELOCITY = 1.198E+03 CM/S  
 TOTAL DEPOSITION RATE = 2.520E-06 G/CM\*\*2/S  
 GAS-PHASE MOLE FRACTIONS  

|         |             |      |             |       |             |
|---------|-------------|------|-------------|-------|-------------|
| H2      | = 4.982E-06 | H    | = 2.260E-08 | N2    | = 1.305E-09 |
| N       | = 1.304E-13 | NH   | = 1.269E-09 | NH2   | = 9.969E-06 |
| NNH     | = 5.472E-11 | N2H2 | = 1.440E-09 | N2H3  | = 4.682E-11 |
| N2H4    | = 1.786E-12 | HF   | = 8.362E-02 | F     | = 4.476E-11 |
| SIF4    | = 1.168E-01 | SIF3 | = 1.376E-10 | SIHF3 | = 7.614E-11 |
| SIF3NH2 | = 3.901E-10 | NH3  | = 7.995E-01 |       |             |

 SURFACE SITE FRACTIONS  

|             |             |               |             |           |             |
|-------------|-------------|---------------|-------------|-----------|-------------|
| HN_SIF(S)   | = 5.536E-02 | F3SI_NH2(S)   | = 2.586E-04 | F2SINH(S) | = 1.845E-02 |
| H2NFSINH(S) | = 2.241E-04 | HN(FSINH)2(S) | = 4.482E-04 | HN_NH2(S) | = 9.253E-01 |

 BULK SPECIES DEPOSITION RATES (MOL/CM\*\*2/S)  

|       |             |      |             |
|-------|-------------|------|-------------|
| SI(D) | = 5.390E-08 | N(D) | = 7.186E-08 |
|-------|-------------|------|-------------|

  
 X = 2.000E+01 CM  
 RESIDENCE TIME = 1.671E-02 S  
 TEMPERATURE = 1713.0 K  
 GAS DENSITY = 4.817E-07 G/CM\*\*3  
 PRESSURE = 1.988E+00 TORR  
 VELOCITY = 1.237E+03 CM/S  
 TOTAL DEPOSITION RATE = 2.099E-06 G/CM\*\*2/S  
 GAS-PHASE MOLE FRACTIONS  

|         |             |      |             |       |             |
|---------|-------------|------|-------------|-------|-------------|
| H2      | = 9.413E-06 | H    | = 2.285E-08 | N2    | = 1.308E-08 |
| N       | = 1.190E-12 | NH   | = 6.085E-09 | NH2   | = 1.873E-05 |
| NNH     | = 2.604E-10 | N2H2 | = 6.753E-09 | N2H3  | = 1.879E-10 |
| N2H4    | = 6.517E-12 | HF   | = 1.486E-01 | F     | = 1.576E-10 |
| SIF4    | = 9.671E-02 | SIF3 | = 1.262E-10 | SIHF3 | = 1.566E-10 |
| SIF3NH2 | = 8.750E-10 | NH3  | = 7.546E-01 |       |             |

 SURFACE SITE FRACTIONS  

|             |             |               |             |           |             |
|-------------|-------------|---------------|-------------|-----------|-------------|
| HN_SIF(S)   | = 4.900E-02 | F3SI_NH2(S)   | = 2.153E-04 | F2SINH(S) | = 1.633E-02 |
| H2NFSINH(S) | = 2.108E-04 | HN(FSINH)2(S) | = 4.217E-04 | HN_NH2(S) | = 9.338E-01 |

 BULK SPECIES DEPOSITION RATES (MOL/CM\*\*2/S)  

|       |             |      |             |
|-------|-------------|------|-------------|
| SI(D) | = 4.488E-08 | N(D) | = 5.984E-08 |
|-------|-------------|------|-------------|

X = 3.000E+01 CM  
 RESIDENCE TIME = 2.469E-02 S  
 TEMPERATURE = 1713.0 K  
 GAS DENSITY = 4.572E-07 G/CM\*\*3  
 PRESSURE = 1.981E+00 TORR  
 VELOCITY = 1.270E+03 CM/S  
 TOTAL DEPOSITION RATE = 1.761E-06 G/CM\*\*2/S  
 GAS-PHASE MOLE FRACTIONS  

|         |             |      |             |       |             |
|---------|-------------|------|-------------|-------|-------------|
| H2      | = 1.348E-05 | H    | = 2.328E-08 | N2    | = 4.567E-08 |
| N       | = 3.905E-12 | NH   | = 1.414E-08 | NH2   | = 2.661E-05 |
| NNH     | = 5.902E-10 | N2H2 | = 1.526E-08 | N2H3  | = 3.958E-10 |
| N2H4    | = 1.326E-11 | HF   | = 2.002E-01 | F     | = 3.163E-10 |
| SIF4    | = 8.074E-02 | SIF3 | = 1.116E-10 | SIHF3 | = 2.210E-10 |
| SIF3NH2 | = 1.325E-09 | NH3  | = 7.190E-01 |       |             |

 SURFACE SITE FRACTIONS  

|             |             |               |             |           |             |
|-------------|-------------|---------------|-------------|-----------|-------------|
| HN_SIF(S)   | = 4.329E-02 | F3SI_NH2(S)   | = 1.807E-04 | F2SINH(S) | = 1.443E-02 |
| H2NFSINH(S) | = 2.002E-04 | HN(FSINH)2(S) | = 4.004E-04 | HN_NH2(S) | = 9.415E-01 |

 BULK SPECIES DEPOSITION RATES (MOL/CM\*\*2/S)  

|       |             |      |             |
|-------|-------------|------|-------------|
| SI(D) | = 3.765E-08 | N(D) | = 5.020E-08 |
|-------|-------------|------|-------------|

  
 X = 4.000E+01 CM  
 RESIDENCE TIME = 3.247E-02 S  
 TEMPERATURE = 1713.0 K  
 GAS DENSITY = 4.372E-07 G/CM\*\*3  
 PRESSURE = 1.974E+00 TORR  
 VELOCITY = 1.299E+03 CM/S  
 TOTAL DEPOSITION RATE = 1.486E-06 G/CM\*\*2/S  
 GAS-PHASE MOLE FRACTIONS  

|         |             |      |             |       |             |
|---------|-------------|------|-------------|-------|-------------|
| H2      | = 1.731E-05 | H    | = 2.387E-08 | N2    | = 1.064E-07 |
| N       | = 8.402E-12 | NH   | = 2.470E-08 | NH2   | = 3.384E-05 |
| NNH     | = 1.019E-09 | N2H2 | = 2.631E-08 | N2H3  | = 6.540E-10 |
| N2H4    | = 2.150E-11 | HF   | = 2.418E-01 | F     | = 5.058E-10 |
| SIF4    | = 6.786E-02 | SIF3 | = 9.853E-11 | SIHF3 | = 2.727E-10 |
| SIF3NH2 | = 1.733E-09 | NH3  | = 6.903E-01 |       |             |

 SURFACE SITE FRACTIONS  

|             |             |               |             |           |             |
|-------------|-------------|---------------|-------------|-----------|-------------|
| HN_SIF(S)   | = 3.818E-02 | F3SI_NH2(S)   | = 1.524E-04 | F2SINH(S) | = 1.273E-02 |
| H2NFSINH(S) | = 1.916E-04 | HN(FSINH)2(S) | = 3.831E-04 | HN_NH2(S) | = 9.484E-01 |

 BULK SPECIES DEPOSITION RATES (MOL/CM\*\*2/S)  

|       |             |      |             |
|-------|-------------|------|-------------|
| SI(D) | = 3.177E-08 | N(D) | = 4.236E-08 |
|-------|-------------|------|-------------|

  
 X = 5.000E+01 CM  
 RESIDENCE TIME = 4.009E-02 S  
 TEMPERATURE = 1713.0 K  
 GAS DENSITY = 4.206E-07 G/CM\*\*3  
 PRESSURE = 1.967E+00 TORR  
 VELOCITY = 1.325E+03 CM/S  
 TOTAL DEPOSITION RATE = 1.259E-06 G/CM\*\*2/S  
 GAS-PHASE MOLE FRACTIONS  

|         |             |      |             |       |             |
|---------|-------------|------|-------------|-------|-------------|
| H2      | = 2.100E-05 | H    | = 2.460E-08 | N2    | = 2.009E-07 |
| N       | = 1.441E-11 | NH   | = 3.716E-08 | NH2   | = 4.057E-05 |
| NNH     | = 1.529E-09 | N2H2 | = 3.951E-08 | N2H3  | = 9.524E-10 |
| N2H4    | = 3.090E-11 | HF   | = 2.758E-01 | F     | = 7.160E-10 |
| SIF4    | = 5.734E-02 | SIF3 | = 8.680E-11 | SIHF3 | = 3.148E-10 |
| SIF3NH2 | = 2.100E-09 | NH3  | = 6.668E-01 |       |             |

 SURFACE SITE FRACTIONS  

|             |             |               |             |           |             |
|-------------|-------------|---------------|-------------|-----------|-------------|
| HN_SIF(S)   | = 3.362E-02 | F3SI_NH2(S)   | = 1.292E-04 | F2SINH(S) | = 1.121E-02 |
| H2NFSINH(S) | = 1.844E-04 | HN(FSINH)2(S) | = 3.688E-04 | HN_NH2(S) | = 9.545E-01 |

 BULK SPECIES DEPOSITION RATES (MOL/CM\*\*2/S)  

|       |             |      |             |
|-------|-------------|------|-------------|
| SI(D) | = 2.692E-08 | N(D) | = 3.590E-08 |
|-------|-------------|------|-------------|

X = 6.000E+01 CM  
 RESIDENCE TIME = 4.757E-02 S  
 TEMPERATURE = 1713.0 K  
 GAS DENSITY = 4.068E-07 G/CM\*\*3  
 PRESSURE = 1.960E+00 TORR  
 VELOCITY = 1.347E+03 CM/S  
 TOTAL DEPOSITION RATE = 1.071E-06 G/CM\*\*2/S  
 GAS-PHASE MOLE FRACTIONS  

|         |             |      |             |       |             |
|---------|-------------|------|-------------|-------|-------------|
| H2      | = 2.462E-05 | H    | = 2.549E-08 | N2    | = 3.337E-07 |
| N       | = 2.153E-11 | NH   | = 5.108E-08 | NH2   | = 4.693E-05 |
| NNH     | = 2.110E-09 | N2H2 | = 5.460E-08 | N2H3  | = 1.285E-09 |
| N2H4    | = 4.127E-11 | HF   | = 3.038E-01 | F     | = 9.395E-10 |
| SIF4    | = 4.867E-02 | SIF3 | = 7.645E-11 | SIHF3 | = 3.494E-10 |
| SIF3NH2 | = 2.429E-09 | NH3  | = 6.474E-01 |       |             |

 SURFACE SITE FRACTIONS  

|             |             |               |             |           |             |
|-------------|-------------|---------------|-------------|-----------|-------------|
| HN_SIF(S)   | = 2.955E-02 | F3SI_NH2(S)   | = 1.099E-04 | F2SINH(S) | = 9.851E-03 |
| H2NFSINH(S) | = 1.784E-04 | HN(FSINH)2(S) | = 3.568E-04 | HN_NH2(S) | = 9.600E-01 |

 BULK SPECIES DEPOSITION RATES (MOL/CM\*\*2/S)  

|       |             |      |             |
|-------|-------------|------|-------------|
| SI(D) | = 2.290E-08 | N(D) | = 3.053E-08 |
|-------|-------------|------|-------------|

 Total CPUtime (sec): 0.09375

## 7. REFERENCES

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